Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:10 PM GMT

PDB ID	:	1SH5
Title	:	Crystal structure of actin-binding domain of mouse plectin
Authors	:	Sevcik, J.; Urbanikova, L.
Deposited on	:	2004-02-25
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

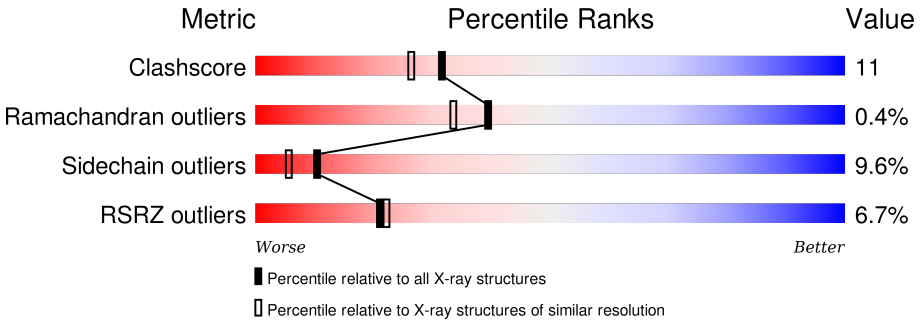
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	245	7% 68% 20% 6% 5%
1	B	245	5% 70% 21% • • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8252 atoms, of which 4226 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Plectin 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	H	N	O	S	138	0	0
			3844	1209	1925	350	353	7			
1	B	232	Total	C	H	N	O	S	138	0	0
			3844	1209	1925	350	353	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q9QXS1
A	2	SER	-	CLONING ARTIFACT	UNP Q9QXS1
A	3	HIS	-	CLONING ARTIFACT	UNP Q9QXS1
A	4	MET	-	CLONING ARTIFACT	UNP Q9QXS1
A	5	GLU	-	CLONING ARTIFACT	UNP Q9QXS1
A	6	PHE	-	CLONING ARTIFACT	UNP Q9QXS1
A	244	GLU	-	CLONING ARTIFACT	UNP Q9QXS1
A	245	PHE	-	CLONING ARTIFACT	UNP Q9QXS1
B	1	GLY	-	CLONING ARTIFACT	UNP Q9QXS1
B	2	SER	-	CLONING ARTIFACT	UNP Q9QXS1
B	3	HIS	-	CLONING ARTIFACT	UNP Q9QXS1
B	4	MET	-	CLONING ARTIFACT	UNP Q9QXS1
B	5	GLU	-	CLONING ARTIFACT	UNP Q9QXS1
B	6	PHE	-	CLONING ARTIFACT	UNP Q9QXS1
B	244	GLU	-	CLONING ARTIFACT	UNP Q9QXS1
B	245	PHE	-	CLONING ARTIFACT	UNP Q9QXS1

- Molecule 2 is water.

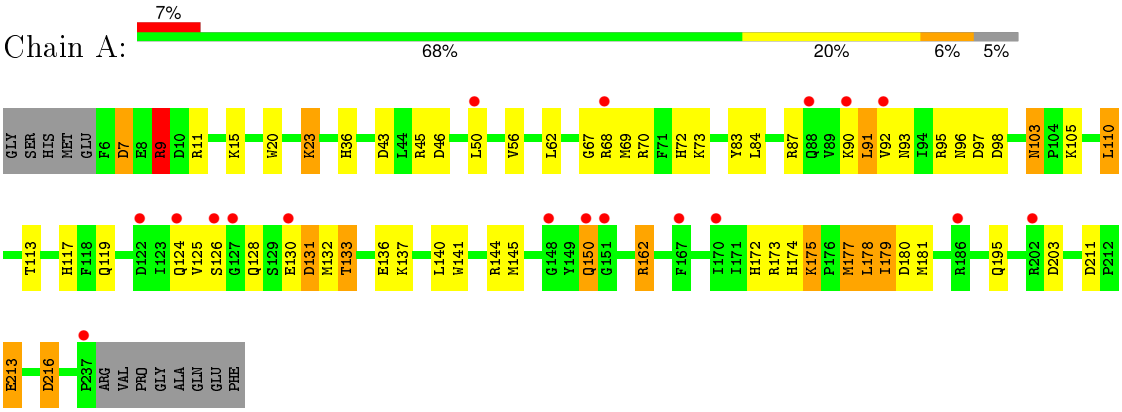
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	96	Total	H	O	192	0
			288	192	96		
2	B	92	Total	H	O	184	0
			276	184	92		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

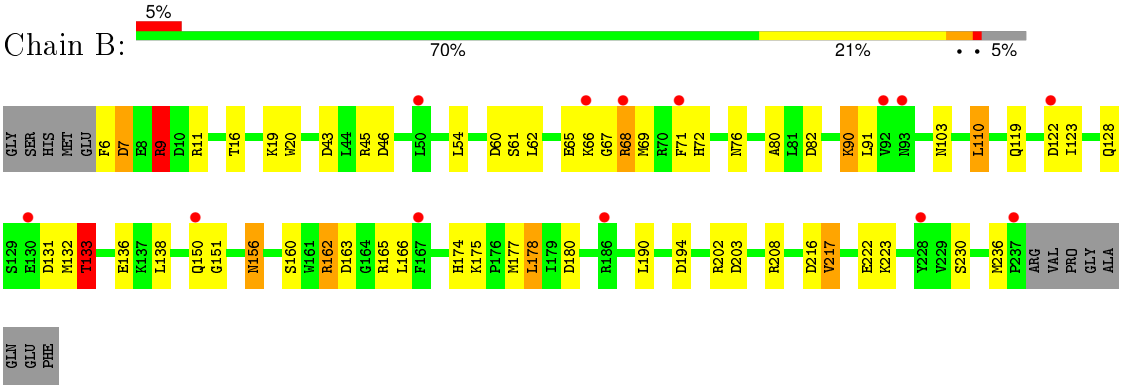
- Molecule 1: Plectin 1

Chain A:



- Molecule 1: Plectin 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.31Å 108.92Å 63.75Å 90.00° 115.25° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 19.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-2.00) 91.8 (19.97-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.151 , 0.194 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.1	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 47777 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8252	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	1.17	2/1957 (0.1%)	1.25	17/2643 (0.6%)
1	B	1.22	9/1957 (0.5%)	1.33	24/2643 (0.9%)
All	All	1.19	11/3914 (0.3%)	1.29	41/5286 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	ARG	CD-NE	-9.77	1.29	1.46
1	A	9	ARG	CD-NE	-7.49	1.33	1.46
1	B	9	ARG	CZ-NH2	-6.67	1.24	1.33
1	B	177	MET	CG-SD	6.54	1.98	1.81
1	B	222	GLU	CD-OE1	-6.29	1.18	1.25
1	A	56	VAL	CB-CG1	-6.07	1.40	1.52
1	B	80	ALA	CA-CB	5.33	1.63	1.52
1	B	230	SER	CB-OG	-5.21	1.35	1.42
1	B	19	LYS	CE-NZ	-5.11	1.36	1.49
1	B	223	LYS	CD-CE	5.06	1.63	1.51
1	B	222	GLU	CD-OE2	-5.02	1.20	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	9	ARG	NE-CZ-NH2	-25.05	107.77	120.30
1	A	9	ARG	NE-CZ-NH2	-21.70	109.45	120.30
1	B	9	ARG	NE-CZ-NH1	19.02	129.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	9	ARG	NE-CZ-NH1	14.50	127.55	120.30
1	B	203	ASP	CB-CG-OD2	10.88	128.09	118.30
1	B	11	ARG	NE-CZ-NH1	-10.37	115.12	120.30
1	A	45	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	A	203	ASP	CB-CG-OD2	8.31	125.78	118.30
1	B	163	ASP	CB-CG-OD2	8.23	125.70	118.30
1	B	46	ASP	CB-CG-OD1	8.15	125.64	118.30
1	A	46	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	98	ASP	CB-CG-OD1	7.47	125.02	118.30
1	A	11	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	B	180	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	7	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	11	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	B	45	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	B	60	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	203	ASP	CB-CG-OD1	-6.47	112.47	118.30
1	B	16	THR	CA-CB-OG1	6.36	122.36	109.00
1	B	133	THR	N-CA-CB	-6.22	98.49	110.30
1	B	7	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	131	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	97	ASP	CB-CG-OD2	6.13	123.81	118.30
1	B	82	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	43	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	217	VAL	CG1-CB-CG2	5.80	120.17	110.90
1	B	165	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	11	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	A	180	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	43	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	194	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	110	LEU	CB-CG-CD2	5.52	120.38	111.00
1	B	223	LYS	CD-CE-NZ	-5.46	99.14	111.70
1	A	216	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	122	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	131	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	177	MET	CG-SD-CE	5.13	108.41	100.20
1	B	45	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	45	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	B	110	LEU	CB-CG-CD2	5.01	119.52	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	151	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1919	1925	1916	51	0
1	B	1919	1925	1916	32	0
2	A	96	192	0	13	0
2	B	92	184	0	8	0
All	All	4026	4226	3832	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:CE	1:A:69:MET:SD	2.03	1.47
1:B:65:GLU:H	1:B:76:ASN:HD21	1.15	0.94
1:B:162:ARG:NH1	1:B:216:ASP:OD1	2.05	0.89
1:A:213:GLU:HG3	2:A:329:HOH:O	1.73	0.89
1:B:156:ASN:HD21	1:B:160:SER:H	1.25	0.84
1:A:23:LYS:HD3	2:A:339:HOH:O	1.77	0.83
1:A:23:LYS:CD	2:A:339:HOH:O	2.28	0.81
1:A:23:LYS:HE3	2:A:339:HOH:O	1.81	0.79
1:B:133:THR:HG22	1:B:136:GLU:H	1.47	0.79
1:A:7:ASP:OD1	1:A:9:ARG:HD3	1.86	0.75
1:A:162:ARG:NH2	1:A:216:ASP:OD1	2.19	0.75
1:A:15:LYS:NZ	1:A:211:ASP:OD2	2.14	0.74
2:A:290:HOH:O	1:B:133:THR:HG21	1.89	0.71
1:B:20:TRP:HE1	1:B:119:GLN:HE22	1.36	0.71
1:A:23:LYS:CE	2:A:339:HOH:O	2.39	0.70
1:A:124:GLN:HA	1:A:128:GLN:NE2	2.07	0.68
1:A:7:ASP:OD1	1:A:9:ARG:CD	2.42	0.68
1:A:179:ILE:HD11	1:A:181:MET:SD	2.34	0.68
1:B:202:ARG:HD2	2:B:297:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HH21	1:A:162:ARG:CG	2.08	0.65
1:A:20:TRP:HE1	1:A:119:GLN:HE22	1.44	0.65
1:A:162:ARG:HH21	1:A:162:ARG:HG2	1.63	0.64
1:A:125:VAL:O	1:A:128:GLN:HG3	1.99	0.63
1:A:133:THR:HG22	1:A:136:GLU:H	1.64	0.62
1:B:20:TRP:HE1	1:B:119:GLN:NE2	1.96	0.62
1:B:67:GLY:HA3	1:B:72:HIS:CD2	2.34	0.62
1:A:69:MET:H	1:A:72:HIS:HD2	1.48	0.61
1:A:126:SER:O	1:A:144:ARG:NH2	2.30	0.59
1:A:145:MET:CE	1:A:174:HIS:CE1	2.86	0.58
1:A:20:TRP:HE1	1:A:119:GLN:NE2	2.01	0.57
1:B:156:ASN:HD22	1:B:156:ASN:C	2.08	0.57
1:B:174:HIS:CD2	1:B:236:MET:HG2	2.40	0.56
1:A:175:LYS:HB3	1:A:178:LEU:HD22	1.87	0.56
1:B:162:ARG:CG	1:B:162:ARG:HH11	2.18	0.56
1:B:175:LYS:HE3	2:B:282:HOH:O	2.06	0.55
1:A:145:MET:HE1	1:A:174:HIS:CE1	2.42	0.54
1:B:71:PHE:CB	2:B:288:HOH:O	2.55	0.53
1:A:141:TRP:O	1:A:145:MET:HG2	2.07	0.53
1:A:213:GLU:CG	2:A:329:HOH:O	2.43	0.53
1:A:36:HIS:HD2	2:A:307:HOH:O	1.92	0.53
1:A:213:GLU:CD	1:A:213:GLU:H	2.13	0.52
1:A:131:ASP:HB2	1:B:90:LYS:NZ	2.24	0.52
1:A:133:THR:HG21	2:B:312:HOH:O	2.10	0.52
1:A:9:ARG:HD2	2:A:331:HOH:O	2.09	0.52
1:A:211:ASP:HB3	1:A:213:GLU:OE1	2.10	0.51
1:B:65:GLU:H	1:B:76:ASN:ND2	1.97	0.51
1:B:71:PHE:HB2	2:B:288:HOH:O	2.11	0.51
1:B:7:ASP:OD1	1:B:9:ARG:CD	2.58	0.51
1:A:145:MET:HE2	1:A:174:HIS:CE1	2.47	0.50
1:A:172:HIS:CD2	1:A:181:MET:HG2	2.46	0.50
1:A:67:GLY:HA3	1:A:72:HIS:CD2	2.46	0.49
1:B:174:HIS:HE1	2:B:282:HOH:O	1.94	0.49
1:A:132:MET:CE	1:A:137:LYS:HG2	2.42	0.49
1:B:67:GLY:C	1:B:72:HIS:CD2	2.87	0.48
1:A:213:GLU:HG3	2:A:306:HOH:O	2.14	0.47
1:B:61:SER:O	1:B:62:LEU:HD23	2.14	0.47
1:A:83:TYR:CZ	1:A:87:ARG:HD2	2.49	0.47
1:A:179:ILE:CD1	1:A:181:MET:SD	3.03	0.46
1:A:23:LYS:HG2	2:A:295:HOH:O	2.16	0.46
1:B:7:ASP:OD1	1:B:9:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:PHE:HB3	2:B:288:HOH:O	2.16	0.45
1:A:145:MET:CE	1:A:174:HIS:HE1	2.30	0.45
1:B:7:ASP:OD1	1:B:9:ARG:HD3	2.16	0.45
1:A:92:VAL:O	1:A:93:ASN:HB2	2.16	0.45
1:B:68:ARG:N	1:B:72:HIS:HD2	2.16	0.44
1:B:175:LYS:HB2	1:B:178:LEU:HD22	1.99	0.44
1:A:83:TYR:CE2	1:A:87:ARG:HD2	2.52	0.44
1:B:67:GLY:CA	1:B:72:HIS:CD2	3.01	0.44
1:A:87:ARG:NH1	1:A:117:HIS:NE2	2.66	0.43
1:A:73:LYS:HD3	2:A:322:HOH:O	2.18	0.43
1:B:90:LYS:CD	1:B:90:LYS:H	2.30	0.43
1:A:91:LEU:HD12	1:A:113:THR:HG21	2.00	0.43
1:B:6:PHE:N	2:B:323:HOH:O	2.51	0.43
1:A:103:ASN:HD22	1:A:103:ASN:C	2.23	0.42
1:A:124:GLN:HA	1:A:128:GLN:HE22	1.81	0.42
1:A:7:ASP:OD1	1:A:9:ARG:HD2	2.18	0.42
1:A:36:HIS:HE1	2:A:318:HOH:O	2.02	0.41
1:B:128:GLN:HA	1:B:132:MET:HE1	2.02	0.41
1:B:69:MET:H	1:B:72:HIS:HD2	1.67	0.41
1:B:123:ILE:HD13	1:B:138:LEU:HD13	2.02	0.41
1:A:172:HIS:HB2	1:A:179:ILE:CG1	2.51	0.41
1:A:62:LEU:HD21	1:A:83:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	230/245 (94%)	225 (98%)	3 (1%)	2 (1%)	21 13
1	B	230/245 (94%)	228 (99%)	2 (1%)	0	100 100
All	All	460/490 (94%)	453 (98%)	5 (1%)	2 (0%)	39 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	96	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	213/223 (96%)	189 (89%)	24 (11%)	7 4
1	B	213/223 (96%)	196 (92%)	17 (8%)	15 9
All	All	426/446 (96%)	385 (90%)	41 (10%)	10 6

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	23	LYS
1	A	50	LEU
1	A	68	ARG
1	A	70	ARG
1	A	84	LEU
1	A	90	LYS
1	A	91	LEU
1	A	95	ARG
1	A	103	ASN
1	A	105	LYS
1	A	110	LEU
1	A	130	GLU
1	A	133	THR
1	A	140	LEU
1	A	150	GLN
1	A	162	ARG
1	A	173	ARG
1	A	175	LYS
1	A	177	MET
1	A	178	LEU

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Mol	Chain	Res	Type
1	A	179	ILE
1	A	195	GLN
1	A	213	GLU
1	B	9	ARG
1	B	54	LEU
1	B	66	LYS
1	B	68	ARG
1	B	90	LYS
1	B	91	LEU
1	B	103	ASN
1	B	110	LEU
1	B	133	THR
1	B	150	GLN
1	B	156	ASN
1	B	162	ARG
1	B	166	LEU
1	B	178	LEU
1	B	190	LEU
1	B	208	ARG
1	B	217	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	75	GLN
1	A	78	GLN
1	A	93	ASN
1	A	96	ASN
1	A	103	ASN
1	A	119	GLN
1	A	128	GLN
1	A	174	HIS
1	A	187	GLN
1	A	195	GLN
1	B	36	HIS
1	B	48	HIS
1	B	72	HIS
1	B	76	ASN
1	B	78	GLN
1	B	93	ASN
1	B	103	ASN

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Mol	Chain	Res	Type
1	B	119	GLN
1	B	150	GLN
1	B	156	ASN
1	B	187	GLN
1	B	195	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	232/245 (94%)	0.10	18 (7%)	16	17	19, 42, 72, 92	0
1	B	232/245 (94%)	-0.01	13 (5%)	28	29	20, 39, 69, 78	0
All	All	464/490 (94%)	0.05	31 (6%)	21	22	19, 40, 71, 92	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	PRO	4.8
1	B	71	PHE	4.6
1	A	127	GLY	4.4
1	A	237	PRO	4.4
1	A	186	ARG	3.7
1	B	130	GLU	3.6
1	A	150	GLN	3.4
1	A	68	ARG	3.4
1	A	122	ASP	3.3
1	A	167	PHE	3.2
1	B	92	VAL	3.1
1	A	126	SER	3.1
1	B	167	PHE	3.1
1	A	202	ARG	3.0
1	B	150	GLN	2.9
1	B	68	ARG	2.9
1	A	151	GLY	2.9
1	B	93	ASN	2.8
1	A	130	GLU	2.7
1	A	90	LYS	2.7
1	B	122	ASP	2.6
1	B	186	ARG	2.6
1	A	124	GLN	2.5
1	A	170	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	66	LYS	2.4
1	A	92	VAL	2.3
1	A	88	GLN	2.3
1	A	50	LEU	2.1
1	B	50	LEU	2.1
1	B	228	TYR	2.0
1	A	148	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.